Modern nucleon-nucleon interactions and charge-symmetry breaking in nuclei

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Abstract

Coulomb displacement energies, i.e., the differences between the energies of corresponding nuclear states in mirror nuclei, are evaluated using recent models for the nucleon-nucleon (NN) interaction. These modern NN potentials account for breaking of isospin symmetry and reproduce *pp* and *pn* phase shifts accurately. The predictions by these new potentials for the binding of ^{16}O are calculated. A particular focus of our study are effects due to nuclear correlations and charge-symmetry breaking (CSB). We find that the CSB terms in the modern NN interactions substantially reduce the discrepancy between theory and experiment for the Coulomb displacement energies; however, our calculations do not completely explain the Nolen-Schiffer anomaly. Potential sources for the remaining discrepancies are discussed.

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The differences between the energies of corresponding states in mirror nuclei, the so-called Coulomb displacement energies, are due to charge-symmetry breaking (CSB) of the nucleon-nucleon (NN) interaction. If one assumes that the strong part of the nuclear force is charge symmetric, i.e. the strong proton-proton interaction is identical to the interaction between two neutrons, then the Coulomb displacement energies would originate entirely from the electromagnetic interaction between the nucleons. The dominant contribution is the Coulomb repulsion. After accurate experimental data on the charge distribution became available from electron scattering experiments, Hartree-Fock calculations with phenomenological models for the NN interaction like the Skyrme forces were performed which reproduced these measured charge distributions with good accuracy. The Coulomb displacement energies which were evaluated with these Hartree-Fock wave functions, however, underestimated the experimental data by typically seven percent. This has become known as the Nolen-Schiffer anomaly [1]. Many attempts have been made to explain this discrepancy by the inclusion of electromagnetic corrections, many-body correlations beyond the Hartree-Fock approach, or by explicit charge-symmetry breaking terms in the NN interaction [2–6].

During the last few years, a new generation of realistic NN interactions has been developed, which yield very accurate fits of the proton-proton (pp) and proton-neutron (pn) data [7–9]. These new interactions account for isospin symmetry breaking (ISB) and also for CSB (which is a special case of ISB). The long-range part of these interactions is described in terms of the one-pion-exchange model, accounting correctly for the mass difference between the neutral pion, π^0, and the charged pions, $\pi^\pm$. This distinction between the masses of a neutral and charged pions is one origin for ISB in the resulting NN interactions. Moreover, these interactions also account for the mass difference between proton and neutron. This gives rise to a difference in the matrix elements of the meson-exchange diagrams between two protons as compared to two neutrons. Within the one-boson-exchange model, this yields only a very small contribution that breaks charge symmetry.

Besides the latter effect, the Argonne and Bonn potentials (which we will apply here) include additional CSB terms necessary to correctly reproduce the empirical differences in the scattering length and effective range parameters for pp and nn scattering in the $^1S_0$ state. The Argonne V_{18} (AV18) potential [8] is constructed in a (S,T) decomposition (where S and T denote the total spin and isospin of the two interacting nucleons). The local potentials in the $(S=0,T=1)$ channel are adjusted such as to reproduce the $^1S_0$ scattering length for the various isospin projections. This method of constructing CSB potentials implies that the information on CSB from the $^1S_0$ scattering length and effective range parameters is simply extrapolated to channels with $L>0$.

More reliably, the information on CSB in NN partial waves with $L>0$ can be derived from a comprehensive meson-exchange model that includes diagrams beyond the simple one-meson-exchange approximation. Based upon the Bonn Full Model [10], ISB effects due to hadron mass-splitting have carefully been calculated up to partial waves with $J=4$ in ref. [11]. The new high-precision NN potential CDBonn99 [12] includes these ISB effects plus the effects from irreducible $\pi\gamma$ exchange as derived in [13]. The difference between CDBonn99 and CDBonn96 [9] is that the latter takes CSB only in $^1S_0$ into account and not in higher partial waves. Thus, a comparison between CDBonn99 and CDBonn96 demonstrates the effect from CSB in states with $L>0$. This will be useful for our discussion below.

It is the aim of the present work to investigate the predictions by these new poten-

tials for the properties of finite nuclei. Our example nucleus is ^{16}O. In particular, we want to determine the effects of correlations and of CSB by these potentials on the calculated Coulomb displacement energy. One possibility would be to perform self-consistent Brueckner-Hartree-Fock (BHF) calculations and extract the Coulomb displacement energies from the single-particle energies for protons and neutrons. We do not take this approach, for the following reasons: (i) Such self-consistent BHF calculations typically predict the radii for the charge-density distributions too small [14]. This implies that the leading Coulomb contribution to the displacement energy would be overestimated. Also the calculation of the correction terms would be based on single-particle wavefunctions which are localized too much. (ii) BHF calculations are appropriate for short-range correlations. However, long-range correlations involving the admixture of configurations with low excitation energies in the uncorrelated shell-model basis require a more careful treatment. (iii) The BHF single-particle energies do not account for any distribution of the single-particle strength consistent with realistic spectral functions.

For the reasons listed, we take the following approach. We use single-particle wave functions from Hartree-Fock calculations with effective nuclear forces, which yield a good fit to the empirical charge distribution. These wave functions are used to determine the leading Coulomb contribution and corrections like the effects of finite proton size, the electromagnetic spin-orbit interaction, the kinetic energy correction due to the mass difference between proton and neutron, and the effects of vacuum polarization. Actually, for these contributions we use the results by Sato [4]. The first column of our table 2 is taken from table 2 of ref. [4] which includes all the effects just listed.

The correlation effects are taken into account in a two-step procedure. We assume a model space defined in terms of shell-model configurations including oscillator single-particle states up to the 1p0f shell. We use the oscillator parameter $b = 1.76$ fm which is appropriate for ^{16}O. The effects of short-range correlations are calculated by employing an effective interaction, i.e. a $\mathcal{G}$-matrix suitable for the model space. This $\mathcal{G}$-matrix is determined as the solution of the Bethe-Goldstone equation

$$\mathcal{G}(\Omega) = V + V\frac{Q_{\rm mod}}{\Omega - Q_{\rm mod}TQ_{\rm mod}}\mathcal{G}(\Omega)\ , \tag{1}$$

where T is identified with the kinetic energy operator, while V stands for the bare two-body interaction including the Coulomb interaction and accounting for ISB terms in the strong interaction. The Pauli operator $Q_{\rm mod}$ in this Bethe-Goldstone eq.(1) is defined in terms of two-particle harmonic oscillator states $|\alpha\beta>$ by

$$Q_{\rm mod}|\alpha\beta>=\begin{cases} 0 & \text{if } \alpha \text{ or } \beta \text{ from } 0s \text{ or } 0p \text{ shell} \\ 0 & \text{if } \alpha \text{ and } \beta \text{ from } 1s0d \text{ or } 1p0f \text{ shell} \\ |\alpha\beta> & \text{elsewhere} \end{cases} \tag{2}$$

As a first approximation we use the resulting $\mathcal{G}$-matrix elements and evaluate single-particle energies in the BHF approximation ϵ_α. This approximation, which will be denoted as BHF in the discussion below, accounts for short-range correlations, which are described in terms of configurations outside our model space. In a next step we add to this BHF definition of the nucleon self-energy the irreducible terms of second order in $\mathcal{G}$ which account for intermediate two-particle one-hole and one-particle two-hole configurations within the model-space

$$\mathcal{U}_\alpha^{(2)} = \frac{1}{2}\sum_{p_1,p_2,h}\frac{<\alpha h|\mathcal{G}|p_1p_2><p_1p_2|\mathcal{G}|\alpha h>}{\omega-(\epsilon_{p_1}+\epsilon_{p_2}-\epsilon_h)+i\eta}+\frac{1}{2}\sum_{h_1,h_2,p}\frac{<\alpha p|\mathcal{G}|h_1h_2><h_1h_2|\mathcal{G}|\alpha h>}{\omega-(\epsilon_{h_1}+\epsilon_{h_2}-\epsilon_p)-i\eta}\,. \quad (3)$$

Applying the techniques described in [15] we can solve the Dyson equation for the single-particle Greens function $G_{\alpha\beta}(\omega)$

$$G_\alpha(\omega) = g^\alpha(\omega) + g_\alpha(\omega)\mathcal{U}_\alpha^{(2)}(\omega)G_\alpha(\omega) \quad (4)$$

with g_α the BHF approximation for the single-particle Greens function, and determine its Lehmann representation

$$G_\alpha(\omega) = \sum_n \frac{\left|<\Psi_n^{A+1}|a_\alpha^\dagger|\Psi_0>\right|^2}{\omega-(E_n^{A+1}-E_0)+i\eta} + \sum_m \frac{\left|<\Psi_m^{A-1}|a_\alpha|\Psi_0>\right|^2}{\omega-(E_0-E_m^{A-1})-i\eta}\,. \quad (5)$$

This yields directly the energies of the states with $A\pm1$ nucleons we are interested in, as well as the spectroscopic factors for nucleon addition or removal.

Numerical results for the binding energy of ^{16}O and some single-particle properties are listed in table 1. This table contains two columns for each NN interaction considered. The columns labeled "ISB" contain results of calculations in which the ISB terms of the interactions are taken into account. In order to demonstrate the size of these ISB terms we also performed calculations, in which we restored isospin-symmetry of the strong interaction by replacing the pp and nn interactions by the corresponding pn interaction (see columns labeled pn).

It is worth noting that the inclusion of long range correlations by means of the Greens function approach outlined above yields an additional binding energy of around 2 MeV per nucleon for all interactions considered. About 1.5 MeV of these 2 MeV per nucleon can be attributed to the admixture of the low-lying particle-particle states within the model space. This energy would also be included in a BHF calculation using the BHF Pauli operator in the Bethe-Goldstone eq.(1) instead of $Q_{\rm mod}$ defined in (2). An additional 0.5 MeV per nucleon arises from the inclusion of the hole-hole scattering terms in the Greens function approach.

The effects of long range correlations are also very important for the quasiparticle energies. For this quantity, however, the effects of low energy particle-particle and hole-hole contributions tend to cancel each other to a large extent. The inclusion of 2p1h configurations within the model space lowers the proton quasiparticle energy for the $p_{1/2}$ state (using AV18) from -12.12 MeV to -15.38 MeV. If, however, the admixture of 2h1p configurations is also included in the definition of the self-energy, the quasiparticle energy yields -12.54 MeV, close to its original BHF value. Similar cancellations are observed for other states and, also, using other NN interactions.

The Bonn potentials CDBonn96 and CDBonn99 yield around 0.9 MeV per nucleon more binding energy than the Argonne potential AV18. This is to be compared with a difference of 1.2 MeV per nucleon, which has been obtained comparing the results of BHF calculations for these potentials in nuclear matter at saturation density [16]. These energy differences can be related to the fact that the Argonne potential is "stiffer" than the Bonn potential [16,18]. More stiffness creates more correlations. This can be seen from the spectroscopic factors in table 1, which deviate more from unity in the case of AV18 as compared to Bonn.

Including the ISB terms in the NN interaction rather than using the np interaction for all isospin channels has a small but non-negligible effect on the calculated binding energies. The scattering lengths for pp and pn scattering implies an NN interaction which is slightly more attractive in the pn as compared to pp. This small difference translates into about 0.2 MeV per nucleon in ^{16}O.

We finally discuss the effects of correlations and of charge-symmetry breaking in the NN interaction on the calculated Coulomb displacement energies. Results are listed in table 2 for various one-hole and one-particle states relative to ^{16}O. The first column of this table, $C^{(1)}$, contains the results of ref. [4] for the leading Coulomb contributions, the corrections due to the finite proton size, the electromagnetic spin-orbit interaction, the kinetic energy correction due to nucleon mass splitting, and the effects of vacuum polarization. As discussed above, we think that it is more realistic to evaluate these contributions for single-particle wave functions which are derived from Hartree-Fock calculations with phenomenological forces rather than using the wavefunctions derived from a microscopic BHF calculation.

The second and third columns of table 2 list the corrections to the Coulomb displacement energies which originate from the treatment of short-range (δ_{SR}) and long-range correlations (δ_{LR}) discussed above. The correction δ_{SR} has been derived from the differences of BHF single-particle energies for protons and neutrons subtracting the Coulomb displacement energy evaluated in the mean-field approximation

$$\delta_{SR} = \epsilon_i^{BHF}(\text{proton}) - \epsilon_i^{BHF}(\text{neutron}) - \delta_{\text{mean field}} \tag{6}$$

In this case the BHF calculations have been performed with the pn versions of the different interactions, i.e. without any ISB terms. The correction terms δ_{LR} have been evaluated in a similar way from the quasiparticle energies determined in the Greens function approach, subtracting the BHF effects already contained in δ_{SR}. The correction terms δ_{SR} and δ_{LR} include the effects represented by irreducible diagrams of second and higher order in the interaction, in which at least one of the interaction lines represents the Coulomb interaction. In addition they contain the effects of folded diagrams discussed by Tam et al. [6]. We find that the correlation effects are rather weak. The short- and long-range contributions tend to cancel each other. This is true in particular for the one-hole states $p_{3/2}^{-1}$ and $p_{1/2}^{-1}$. The effects of short-range correlations dominate in the case of the particle states, $d_{5/2}$ and $1s_{1/2}$, leading to a total correlation effect around 100 keV in the Coulomb displacement energies. This effect is slightly larger for the Argonne potential than for the Bonn potentials because of the stronger correlations in the case of Argonne.

The contributions to the Coulomb displacement energies caused by the CSB terms in the NN interactions, δ_{CSB}, are listed in the fourth column of table 2. The CDBonn96 potential, which includes CSB only in the $^1S_0$ state to fit the empirical pp and nn scattering lengths, provides the smallest δ_{CSB}. When CSB as derived from a comprehensive meson-exchange model is included in partial waves with $L > 0$, as done in CDBonn99, then the δ_{CSB} contribution about doubles. The Argonne AV18 potential also includes CSB for $L > 0$ and, therefore, produces a relatively large δ_{CSB}. Note, however, that the CSB for $L > 0$ in AV18 is just an extrapolation of what $^1S_0$ needs to fit the pp and nn scattering lengths; it is not based upon theory.

In any case, when a NN potential includes CSB beyond the $^1S_0$ state, then a contribution to the Coulomb displacement energies of about 100 keV is created, while CSB in $^1S_0$ only

generates merely about 50 keV. This demonstrates how important it is to include CSB in all relevant NN partial waves if one wants to discuss a phenomenon like the Nolen-Schiffer anomaly in a proper way.

However, it also turns out that even this carefull consideration of CSB does not fully explain the Nolen-Schiffer anomaly, in our calculations. Our final predictions given in column C^{Tot} of table 2 still differ by about 100 keV from the experimental values. Thus the CSB NN force contribution has cut in half the original discrepancy of about 200 keV.

For the remaining discrepancy, many explanations are possible. First, the nuclear structure part of our calculations may carry some uncertainty. To obtain an idea of how large such uncertainties may be, we compare the results for Coulomb displacement energies using the Skyrme II force and *no CSB* by Sato [4] with the more recent ones by Suzuki *et al.* [17]. For the single-hole state $p_{1/2}^{-1}$, Suzuki's result is larger by 167 keV as compared to Sato; and for the single-particle state $d_{5/2}$, the two calculations differ by 138 keV. Uncertainties of this size can well explain the remaining discrepancies in our results.

Another possibility is that the CSB forces contained in CDBonn99 and AV18 are too weak. Based upon our results, it may be suggestive to conclude that CSB forces of about twice their current strength are needed. Notice, however, that one cannot just add more CSB forces to these potentials. A crucial constraint for any realistic CSB NN force is that it reproduces the empirical difference between the pp and nn $^1S_0$ scattering lengths, $\Delta a_{CSB} = 1.5 \pm 0.5$ fm [2]. The CSB contained in CDBonn99 is based upon nucleon mass-difference effects as obtained in a comprehensive meson-exchange model which completely explains the entire Δa_{CSB} [11] leaving no room for additional CSB contributions.

The only possibility that remains then is to simply ignore the above CSB effects and consider an alternative source for CSB, namely $\rho^0 - \omega$ mixing. Traditionally, it was believed that $\rho^0 - \omega$ mixing causes essentially all CSB in the nuclear force [2]. However, recently some doubt has been cast on this paradigm. Some researchers [20–22] found that $\rho^0 - \omega$ exchange may have a substantial q^2 dependence such as to cause this contribution to nearly vanish in NN. The recent findings of ref. [11] that the empirically known CSB in the nuclear force can be explained solely from nucleon mass splitting (leaving essentially no room for additional CSB contributions from $\rho^0 - \omega$ mixing or other sources) fits well into this new scenario. However, since the issue of the q^2 dependence of $\rho^0 - \omega$ exchange and its impact on NN is by no means settled (see Refs. [23,24] for critical discussions and more references), it is premature to draw any definite conclusions. In any case, for test purposes one may invoke the $\rho^0 - \omega$ mechanism as an alternative.

Note, however, that due to the constraint that the $^1S_0$ Δa_{CSB} be reproduced quantitatively, the $^1S_0$ contribution will most likely not change, no matter what miscroscopic mechanism is assumed for CSB. However, the CSB contributions in partial waves with $L > 0$ may depend sensitively on the underlying mechanism. The CSB force caused by nucleon mass-splitting has essential scalar character, while $\rho^0 - \omega$ exchange is of vector nature. Since we have seen above that the $L > 0$ partial waves produce about 50% of the total CSB effect, higher partial waves may carry the potential for substantial changes. This would be an interesting topic for a future investigation.

In summary, we have compared results for bulk properties of finite nuclei derived from modern models of the nucleon-nucleon interaction. Effects of short-range as well as long-range correlations are taken into account. The different models for the NN interaction are

essentially phase-shift equivalent. Nevertheless they predict differences in the binding energy of ^{16}O up to 1 MeV per nucleon. The main source for this discrepancy could be the local versus non-local description of the pion exchange interaction as discussed in the literature for the deuteron [19] and nuclear matter [18]. The CSB force components contained in the CDBonn99 and AV18 potentials cut in half the discrepancy that is know as the Nolen-Schiffer anomaly. The remainder of the discrepancy may be due to subtle nuclear structure effects left out in our current calculations. The consideration of alternative mechanism for CSB has also the potential to shed light on open issues.

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TABLES

	CDBonn96		CDBonn99		AV18	
	pn	ISB	*pn*	ISB	*pn*	ISB
$\epsilon^{BHF}_{p3/2}$ [MeV]	-17.37	-17.23	-17.39	-17.05	-15.89	-15.58
$\epsilon^{BHF}_{p1/2}$ [MeV]	-13.68	-13.49	-13.71	-13.36	-12.43	-12.12
$\epsilon^{BHF}_{d5/2}$ [MeV]	0.39	0.99	0.36	0.99	1.34	2.07
E^{BHF}/A [MeV]	-4.80	-4.72	-4.81	-4.65	-3.97	-3.82
$\epsilon^{QP}_{p3/2}$ [MeV]	-17.65	-17.52	-17.68	-17.32	-16.14	-15.82
$\epsilon^{QP}_{p1/2}$ [MeV]	-14.23	-14.03	-14.26	-13.88	-12.88	-12.54
$\epsilon^{QP}_{d5/2}$ [MeV]	-0.57	0.05	-0.60	0.03	0.44	1.16
$S_{p3/2}$	.8071	.8089	.8070	.8087	.7867	.7852
$S_{p1/2}$	.7937	.7960	.7936	.7956	.7721	.7745
$S_{d5/2}$	.8460	.8474	.8460	.8472	.8238	.8261
E/A [MeV]	-6.89	-6.70	-6.90	-6.70	-5.94	-5.76

TABLE I. Single-particle properties and binding energy per nucleon of ^{16}O calculated for the potentials CDBonn96, CDBonn99, and AV18. The results in columns ISB are obtained by taking the ISB of these potentials properly into account while for columns *pn* only the *pn* potentials are used throughout ignoring ISB. Results for proton single-particle energies are listed for the BHF approximation (ϵ^{BHF}_{α}) and for the complete Greens function approach (ϵ^{QP}_{α}). For the latter case, also the spectroscopic factors S_{α} are listed. The total energies per nucleon (denoted by E^{BHF}/A for BHF and by E/A for the Greens function approach) include a correction for the spurious center of mass motion.

		$C^{(1)}$	δ_{SR}	δ_{LR}	δ_{CSB}	C^{Tot}	Exp
$p_{3/2}^{-1}$	CDBonn96	3205	-44	46	36	3240	3395
	CDBonn99		-44	46	86	3290	
	AV18		-71	47	108	3285	
$p_{1/2}^{-1}$	CDBonn96	3235	-52	37	54	3271	3542
	CDBonn99		-52	37	91	3320	
	AV18		-79	39	103	3297	
$d_{5/2}$	CDBonn96	3135	154	-15	49	3326	3542
	CDBonn99		154	-15	72	3350	
	AV18		187	-18	92	3401	
$1s_{1/2}$	CDBonn96	2905	159	-45	58	3081	3166
	CDBonn99		160	-46	93	3117	
	AV18		198	-47	112	3174	

TABLE II. Coulomb displacement energies for single-hole ($p_{3/2}^{-1}$ and $p_{1/2}^{-1}$) and single-particle states ($d_{5/2}$ and $1s_{1/2}$) around ^{16}O. The single-particle contribution, $C^{(1)}$, is from Sato [4]. Contributions due to short-range correlations, δ_{SR}, long-range correlations inside the model space, δ_{LR}, and due to the charge-symmetry breaking terms in the strong interaction, δ_{CSB}, are calculated for three different NN interactions. The total results for the displacement energies, C^{Tot}, are compared to the experimental data given in the last column. All entries are in keV.